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Computer simulation methods have been used to study spiral crystal growth from multiple dislocation edges. The results showed that after the spiral arms had all interacted once growth proceeded in agreement with the Burton-Cabrera-Frank continuum theory. For small Frank-Read dislocations the existence of a nucleation barrier was shown. Computer simulation studies of simple models of magnetic (binary alloy) lattices with exposed surfaces were also

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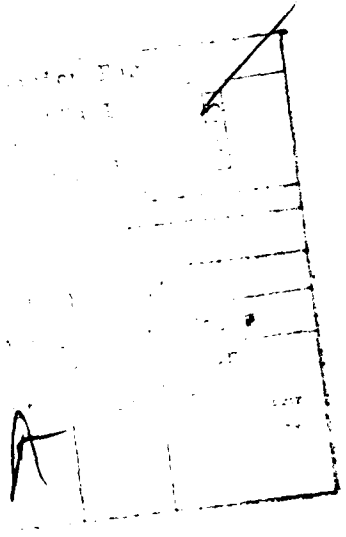
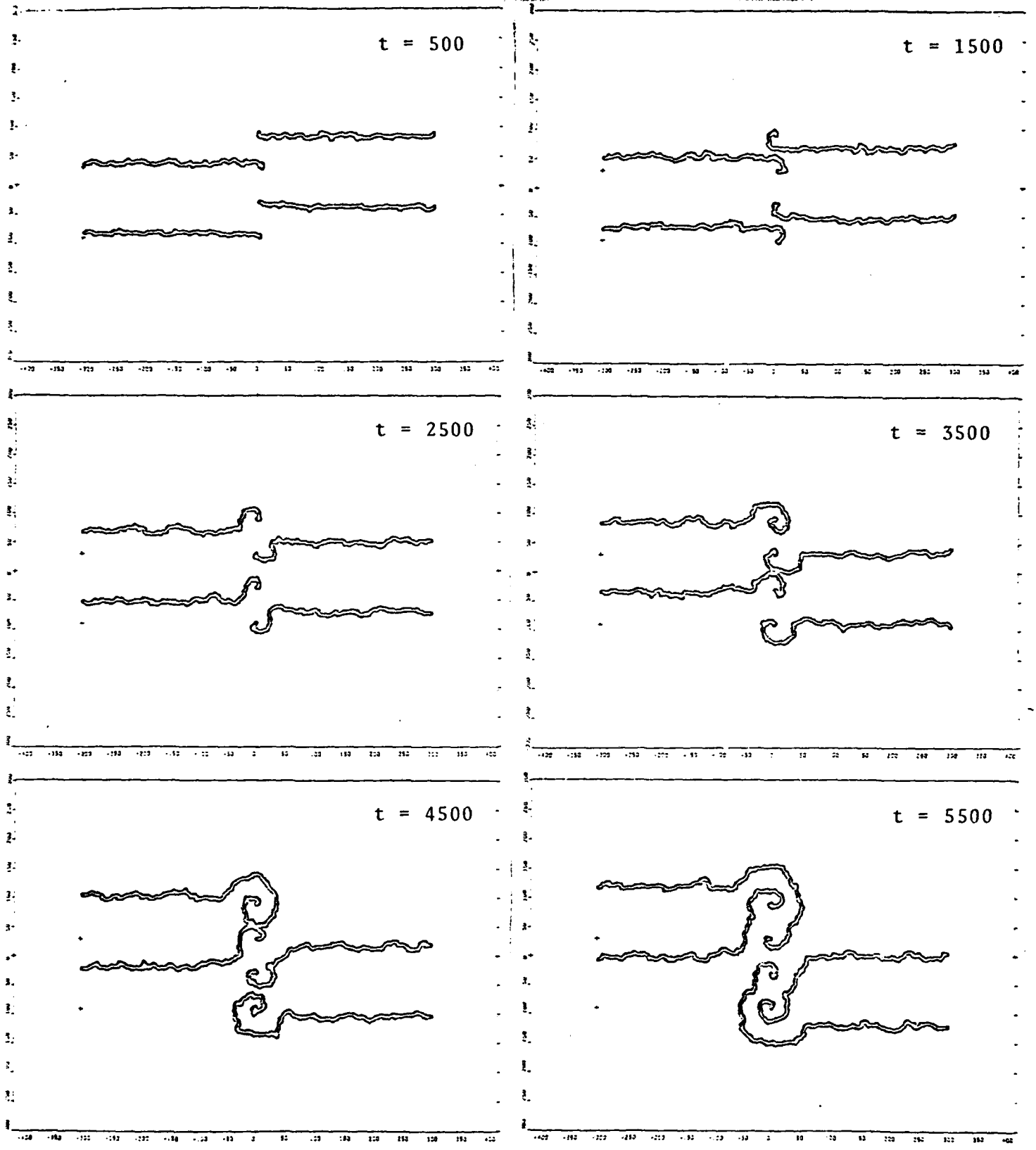
carried out. Surface order-disorder and order-order transitions were studied as a function coupling both below and above the bulk transition surface.



A. Spiral Crystal Growth from Multiple Dislocation Edges

Our goal was to study growth from crystal dislocation edges under conditions where nucleation and surface diffusion were not important factors. Starting with a simple Kossel model, we placed one or more dislocations in the surface with Burgers vector perpendicular to this surface. When a chemical potential difference $\Delta\mu$ was applied, the crystal could begin to grow (spiral) from the dislocation edges. Viewing the crystal from above we could observe growth toward the top or bottom of the face depending upon the sign of the dislocations. Mirror boundary conditions were applied to the sides, but when any part of the growth edge reached the top or the bottom execution was terminated. Overhangs, vacancies, and isolated adatoms were not allowed. Simulations were carried out on L x L surfaces with L typically between 200 and 600. Adatoms were allowed to adsorb or evaporate with equal probability along each dislocation in a given simulation. Most data were obtained for $\varepsilon/kT = 1$ where ε is the bond energy. Interactions were restricted to nearest-neighbor sites. Various combinations of dislocations were studied and the results were compared with earlier simulation data on single spirals. Extensive data were obtained on Frank-Read dislocations (i.e. two largely-superimposed colinear dislocations of opposite sign) with widths between 2 and 150 lattice spacing.

or dislocation widths less than the critical diameter for two-dimensional nucleation, the results showed clear evidence of a nucleation barrier. The dislocation edge would bow out slightly and growth would then cease. The growth edge would fluctuate in shape but would not grow until some characteristic time had passed. For small $\Delta\mu$ and small dislocation widths the metastable growth edge could persist up to 2×10^4 time units! Once growth began, however, the motion of the growth edge was equivalent and the rate varied linearly with $\Delta\mu$ in all cases. We have also studied growth from dislocations which begin on a single vertical line and run alternately to the left and right. The vertical distance between dislocations, Δx, was varied as was the chemical potential difference $\Delta\mu$. Runs were carried out on 600 x 600 lattices and the number of particles added in a 100 x 100 section near the center of the lattice was determined. Limiting case were: a) $\Delta x = 6$, $\Delta\mu/kT = .10$ (for which the critical radius for surface nucleation $r_c \sim 6$; b) $\Delta x = 60$, $\Delta\mu/kT = .30$ (for which $r_c \sim 1.5$). After all spiral arms had interacted at least once the growth increased linearly with time; the net activity was consistent with the Burton-Cabrera-Frank continuum theory.



Sample "snapshots" of the projection of the growth edges as a function of time for $J/kT = 1.0$ $\Delta\mu/kT = 0.3$. The initial distance between dislocations is 60 lattice spacings.

B. Phase Transitions and Order at Surfaces

We have studied surface order-disorder transitions using an Ising-binary alloy model on a simple cubic lattice. Lattices were made up of L x L layers with periodic boundary conditions; the lattices were M layers thick with free surfaces at the top and bottom. Monte Carlo computer simulation studies were made using constant interactions within the bulk but varying the interactions within the surface layers. Finite size effects proved important and both 20 x 20 x 10 and 50 x 50 x 20 lattices were examined so that the effects of finite size could be determined. Our data showed that near to the bulk transition the center of a solid only 10 layers thick showed deviations from the infinite lattice critical behavior. The 20 layer thick lattices did not show this behavior for temperatures which were not so close to a transition that they were not dominated by statistical fluctuations. Up to 3×10^7 μ-trials were carried out in order to obtain data of good quality. For small surface coupling J_s the surface disordered with the bulk as the temperature was raised. For surface coupling J, we found ferromagnetic surface critical temperatures (surface segregation) which exceeded the bulk ordering temperature. For $J_s/J>1.2$. When the surface coupling is zero or slightly negative the surface is dragged along with the bulk. For $J_s<J$ the surface magnetization continued to show the same

asymptotic critical behavior but with greatly reduced amplitude. Values of the surface magnetization as low as 0.04 were clearly observable in spite of fluctuations. The critical behavior of the surface magnetization was given by $m_1 \propto (T-T_c)^{\beta_1}$ with $\beta_1 = 0.080 \pm 0.05$. For $J_s/J < 1.9 \pm 0.1$ the surface orders antiferromagnetically (surface reconstruction) above the bulk critical temperature and disorders at higher temperatures which depend upon J_s/J. For $J_s/J > -1.9 \pm 0.1$ the surface orders ferromagnetically when the bulk orders; but for $-1.9 \leq J_s/J \leq -0.25$ a second phase transition occurs as the temperature is lowered to an antiferromagnetic surface state (but the bulk is not affected). This surface antiferromagnetic transition seems to be first order at low temperature but is clearly second order above the bulk transition temperature. We have not yet been able to determine if the order changes at the surface-bulk multicritical point or at some lower temperature. Cross-section profiles showed that in all cases the bulk behavior persisted up to within two- or three-layers from the surface, even when the bulk was ferromagnetic and the surface antiferromagnetic.